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o an reverse side if necessary and identify by block number) The topics investigated experimentally and theoretically by the Pittsburgh Atomic Sciences Institute with applications to high power laser development and atmospheric IR backgrounds are enumerated. Reports containing the detailed scientific progress in these studies are cited. Finally, a list of the journal articles describing the results of the programs, with full references, is given.

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FINAL REPORT

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PROGRAM CODE NUMBER:

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NAME OF CONTRACTOR:

Department of Physics and Astronomy

and Department of Chemistry University of Pittsburgh Pittsburgh, PA 15260

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PROJECT SCLENTIST:

M. A. Biondi, Director

Professor of Physics

Telephone: Area Code 412

624-4354

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The views and conclusions contained in this document are those of the authors and should not be interpreted as necessarily representing the official policies, either expressed or implied, of the Advanced Research Projects Agency or the U.S. Government.

I. Scope of the Research Programs

During the period of this contract, July 1, 1975 - May 15, 1980, the Pittsburgh Atomic Sciences Institute (PASI) carried out experimental and theoretical studies of atomic collision processes with applications to high-power laser developments and atmospheric IR radiation backgrounds. The detailed scientific progress has been described in a series of semiannual reports. PASI Technical Progress Summaries Nos. 19-25.

The topics investigated include the following experimental programs.

- 1. Laser Ion-Molecule Reaction Rates
- 2. Energy Transfer Processes of Laser Interest
- 3. Dissociative Recombination and Dissociative Excitation
- 4. Metal Atom Chemi-excitation
- 5. Infrared Chemiluminescence
- 5. Atmospheric Particulate Technology

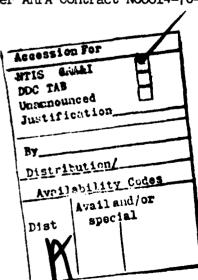
The topics under theoretical investigation were:

- 1. Charge Transfer
- 2. Rotational Excitation of Diatomic Molecules
- 3. Ion Velocity Distributions in Drift Tubes
- 5. V → E Energy Transfer
 5. Ion-Ton Francisco -. Excimer Potential Curves

The results of these studies have been fully described in the journal publications listed in the next section.

II. Publications by PASI under the Contract

The results of the researches carried out in the various programs described in Sec. I have been described in articles in a number of journal publications. The following list gives the title, authors and journal reference for the publications under ARPA Contract NOO014-76-C-0098:



Publications

Calculations of Ion-Atom Interactions Relating to Resonant Charge-Transfer Collisions, J. N. Bardsley, Phys. Rev. A <u>11</u>, 1911, 1975.

Computation of Speed Distributions for Ions in Drift Tubes, J. N. Bardsley and S. L. Lin, J. Phys. B 8, L461, 1975.

Pseudopotential Calculations for Na, , Na, and Na, , J. N. Bardsley, B. R. Junker and D. W. Norcross, Chem. Phys. Lett. 37, 2502, 1976.

Electron-Positron Pair Bound to an Extended Dipole, J. N. Bardsley, W. Brandt, A. Dupasquier and B. R. Junker, Phys. Rev. B <u>13</u>, 4175, 1976.

Symmetric Charge Transfer in Low-Energy Ion-Atom Collisions, S. Sinha and J. N. Bardsley, Phys. Rev. A 14, 104, 1976.

Monte Carlo Simulation of Ion Motion in Drift Tubes, S. L. Lin and J. N. Bardsley, J. Chem. Phys. 66,435, 1977.

Calculations of ion-ion recombination at high pressures, J. M. Wadehra and J. N. Bardsley, Appl. Phys. Lett. <u>32</u>, 76, 1978.

Velocity and Energy Relaxation of Ions in Drift Tubes, S. L. Lin, L. A. Viehland, E. A. Mason, J. H. Whealton and J. N. Bardsley, J. Phys. B <u>10</u>, 3567, 1977.

The Null-Event Method in Computer Simulation, S. L. Lin and J. N. Bardsley, Comp. Phys. Comm. 15, 161, 1978.

The Mobility of He[†] Ions in He, Swati Sinha, S. L. Lin and J. N. Bardsley, J. Phys. B 12, 1613, 1979.

Resonant Contributions to Single Charge Transfer between ${\rm He}^{2+}$ and ${\rm He}$, J. N. Bardsley, James S. Cohen and J. M. Wadehra, Phys. Rev. A $\underline{19}$, 2129, 1979.

Molecular Resonance Phenomena, J. N. Bardsley, in Electron-Molecule and Photon-Molecule Collisions, Eds. T. Rescigno, V. McKay and B. Schneider (Plenum, 1979) p. 267.

Cross Sections for the Reaction $0^{-} + 0_{2} + 0_{3}^{-} + 0$ at Relative Kinetic Energies 0.04 - 2 eV, S. L. Lin, J. N. Bardsley, I. Dotan, F. C. Fehsenfeld and D. L. Albritton, Int. J. Mass. Spectrom. Ion Phys., 1979.

Spectroscopic Studies of the Charge Transfer Reaction He⁺ + Hg + He + (Hg⁺) at Thermal Energy", Edward Graham IV, Manfred A. Biondi and Rainer Johnsen, Phys. Rev. A 13, 965, 1976.

Dissociative Recombination in Xenon: Variation of the Total Rate Coefficient and Excited-State Production with Electron Temperature, Y. J. Shiu, M. A. Biondi and D. P. Sipler, Phys. Rev. A 15, 494, 1977.

Dissociative Recombination in Krypton: Dependence of the Total Rate Coefficient and Excited State Production on Electron Temperature, Yueh-Jaw Shiu and Manfred A. Biondi, Phys. Rev. A 16, 1817, 1977.

Publications - cont'd.

Dissociative Recombination in Argon: Dependence of the total rate coefficient and excited-state production on electron temperature, Yueh-Jaw Shiu and Manfred A. Biondi, Phys. Rev. A 17, 868, 1978.

Thermal-Energy Charge Transfer, Quenching and Association Reactions of Doubly Charged Ions in the Rare Gases, Rainer Johnsen and Manfred A. Biondi, Phys. Rev. A 20, 87, 1979.

Ion-Molecule Reactions of He⁺, Ne⁺, N⁺, N₂⁺, N₃⁺, and N₁⁺ Ions with Hg Atoms and Hg Br₂ Molecules at Thermal Energy, Rainer Johnsen and Manfred A. Biondi, J. Chem. Phys. 2 (to be published), 1980.

Charge Transfer of Atomic and Molecular Rare-Gas Ions with Mercury Atoms at Thermal Energy, Rainer Johnsen and Manfred A. Biondi, J. Chem. Phys. (to be published), 1980.

An Automatic Real-Time Detector and Sizer for Submicron Airborne Particulate Matter, W. L. Fite, R. L. Myers, T. M. Barlak, Rev. of Sci. Instr., 1975.

Submicron and Centimicron Particulate Detection Using Surface Ionization, W. L. Fite and R. L. Myers, American Laboratory Magazine, December 1975.

Spatial Separation of Fringe Fields in Quadrupole Mass Filters, W. L. Fite, Rev. Sci. Instr. 47, 326, 1976.

Reactions Between NO⁺ and Metal Atoms Using Magnetically Confined Afterglows, H. H. Lo, L. M. Clendenning and W. L. Fite, J. Chem. Phys. <u>66</u>, 947, 1977.

Hydrogen Chemistry: Perspective on Experiment and Theory, F. Kaufman, in "Atmospheres of the Earth and the Planets", B. M. McCormac, Ed., D. Reidel Publishing Company, Dordrecht, Holland, p. 219 (1975).

Re-evaluation of the BEBO Method, R. M. Jordan and F. Kaufman, J. Chem. Phys. 63, 1691 (1975).

Kinetics of the Reaction OH + D + OD + H, J. J. Margitan and F. Kaufman, Chem. Phys. Lett. 34, 485, 1975.

The Reaction of CO, with Active Nitrogen, W. T. Rawlins and F. Kaufman, J. Chem. Phys. 64, 1128, 1976.

Kinetics of the Reaction Cl + 0_3 + Cl0 + 0_2 , M. S. Zahniser, F. Kaufman and J. G. Anderson, Chem. Phys. Lett. 37, 226, 21976.

Measurements of Ortho-Para Ratio in Gas Phase Hydrogen Atom Recombination, L. P. Walkauskas and F. Kaufman, J. Chem. Phys. <u>64</u>, 3885, 1976.

Flowing Afterglow Studies of Hydronium Ion Clustering Including Diffusion Effects, V. M. Bierbaum, M. F. Golde and F. Kaufman, J. Chem. Phys. 65,2715, 1976/

Fluorescence Lifetime Studies of NO₂: I. Excitation of the Perturbed ²B₂ State Near 600 nm, V. M. Donnelly and F. Kaufman, J. Chem. Phys. <u>66</u>, 4100, 1977.

Characteristics of OI and NI Resonance Line Broadening in Low Pressure Helium Discharge Lamps, W. T. Rawlins and F. Kaufman, J. Quant. Spec. and Rad. Trans. 18, 561, 1977.

Publications - cont'd.

Mechanism of NO₂ Fluorescence Quenching, V. M. Donnelly and F. Kaufman, J. Chem. Phys. 67, 4768, 21977.

The Thermal Rate Constant of Elementary Reactions: Does Specificity of Energy Disposal Require a Concomitant Lowering of its Magnitude? F. Kaufman and R. D. Levine, Chem. Phys. Lett. 54, 407, 1978.

Reply to Comment on Mechanism of NO $_2$ Fluorescence, V. M. Donnelly and F. Kaufman, J. Chem. Phys. $\underline{68}$, 5671, 1978.

Fluorescence Lifetime Studies of NO₂: II. Dependence of the Perturbed ²B₂ State Lifetimes on Excitation Energy, V. M. Donnelly and F. Kaufman, J. Chem. Phys. 69, 1456, 1978.

Dissociation of CH_{ij} and CD_{ij} by Electron Impact: Production of Metastable and High-Rydberg Hydrogen and Carbon Fragments, B. L. Carnahan, T. F. Finn, W. C. Wells and E. C. Zipf, J. Chem. Phys. $\underline{63}$, 1596, 1975.

Translational Spectroscopy of Metastable Fragments Produced by Dissociative Excitation of Atmospheric Gases by Electron Impact: I. Nitrogen, Phys. Rev. 14, 695, 1976.

Translational Spectroscopy of Metastable Fragments Produced by Dissociative Excitation of Atmospheric Gases by Electron Impact: II. Carbon Monoxide, W. C. Wells, W. L. Borst, and E. C. Zipf, Phys. Rev. A 17, 1357, 1978.

On the Excitation of the NO γ -bands in Auroras, T. G. Finn, B. L. Carnahan, and E. C. Zipf, Trans. Am. Geophys. Union, <u>56</u>, 414, 1975.

Translational Spectroscopy of Metastable Fragments Produced by Dissociative Excitation of Atmospheric Gases by Electron Impact. I. Nitrogen, Phys. Rev. 14, 695, 1976.

Dissociative Excitation of H_2 , HD, and D_2 by Electron Impact, B. L. Carnahan and E. C. Zipf, Phys. Rev. $A^2\underline{16}$, 991, 1977.

On the Excitation of Lyman 8 and Balmer α Radiation by Electron Impact Dissociation of Methane, R. W. McLaughlin and E. C. Zipf, Chem. Phys. Lett. 55, 62, 1978.

On the Dissociation of Nitrogen by Electron Impact and EUV Photoabsorption, E. C. Zipf and R. W. McLaughlin, Planet. Space Sci. 26, 449, 1978.

A Study of the Excitation and Radiative Decay of the 3s' ³Do and 3d^o levels of Atomic Oxygen, R. W. McLaughlin, E. C. Zipf, and M. R. Gorman, Planet. Space Sci. <u>27</u>, 719, 1979.

Translational Spectroscopy of Metastable Fragments Produced by Dissociative Excitation of Chlorine, W. C. Wells and E. C. Zipf, J. Chem. Phys. <u>66</u>, 5828, 1977.

The Excitation and Collisional Deactivation of Metastable N(2P) Atoms in Auroras, E. C. Zipf, P. J. Espy, and C. F. Boyle, J. Geophys. Res., 1978.

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